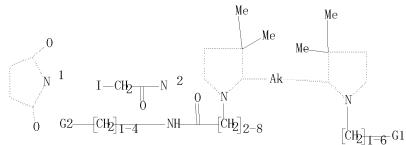
\Rightarrow d his

(FILE 'HOME' ENTERED AT 14:21:25 ON 08 JAN 2009)

FILE 'REGISTRY' ENTERED AT 14:21:39 ON 08 JAN 2009 STRUCTURE UPLOADED 4 S L1 26 S L1 FULL

- L1
- L2 L3
- \Rightarrow d que 13 stat
- STR



G1 S03H, H

G2 [@1], [@2]

Structure attributes must be viewed using STN Express query preparation. 26 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 89 ITERATIONS SEARCH TIME: 00.00.01

26 ANSWERS

 \Rightarrow d 1-26 ide can

- L3ANSWER 1 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN
- RN
- ED
- 1071969-32-8 REGISTRY Entered STN: 11 Nov 2008 INDEX NAME NOT YET ASSIGNED ${\rm CN}$
- FS PROTEIN SEQUENCE; STEREOSEARCH
- ${\rm MF}$ C103 H152 N22 033 S3
- CA
- SR LC STN Files: CA, CAPLUS

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1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3ANSWER 2 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN
- RN
- ED
- 1071969-30-6 REGISTRY Entered STN: 11 Nov 2008 INDEX NAME NOT YET ASSIGNED ${\rm CN}$
- FS PROTEIN SEQUENCE; STEREOSEARCH
- ${\rm MF}$ C102 H147 N19 035 S3
- CA
- SR LC STN Files: CA, CAPLUS

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С02H С02H S Pr-i

> 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 3 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 950890-22-9 REGISTRY
 Entered STN: 18 Oct 2007
 Glycinamide, L-tyrosyl-D-alanyl-L-phenylalanyl-L-α-glutamyl-L-CNisoleucyl-L-isoleucylglycylglycyl-18-amino-5-oxo-3, 9, 12, 15-tetraoxa-6-azaoctadecanoyl-S-[1-[2-[[6-[2-[3-(1-ethyl-1, 3-dihydro-3, 3-dimethyl-5-2]]]])). The standard of the second context of thesulfo-2H-indol-2-ylidene)-1-propen-1-yl]-3, 3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-, inner salt (CA INDEX NAME)
- FS PROTEIN SEQUENCE; STEREOSEARCH
- MF C97 H137 N17 O28 S3
- SR CA
- LC STN Files: CA, CAPLUS

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1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 4 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3

ANSWER 4 OF 26 REGISTRY COPYRIGHT 2009 ACS ON SIN

RN 945985-10-4 REGISTRY

ED Entered STN: 04 Sep 2007

CN 3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-y1)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1, 3-pentadien-1-yl]-1-[(3,5-dinitrophenyl)methyl]-3, 3-dimethyl-5-sulfo-, 2, 2, 2-trifluoroacetate (1:1) (CA INDEX NAME)

OTHER NAMES:

Cy 5Q CN

MF C44 H47 N6 O13 S2 . C2 F3 O2

SR

STN Files: CA, CAPLUS

> CM1

CRN 945985-09-1

CMF C44 H47 N6 013 S2

H03S Me Me CH-CH=CH=CH=CH=CH=S03H
$$(CH_2)_5 - C - NH - CH_2 - CH_2 - N$$

CM2

 $CRN \quad 14477 - 72 - 6$ CMF C2 F3 O2

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 5 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- ANSWER 5 OF 26 REGISTRY COPYRIGHT 2009 ACS ON STN 945985-09-1 REGISTRY
 Entered STN: 04 Sep 2007
 3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-y1)ethy1]amino]-6-oxohexy1]-1,3-dihydro-3,3-dimethy1-5-sulfo-2H-indol-2-ylidene]-1,3-pentadien-1-y1]-1-[(3,5-dinitropheny1)methy1]-3,3-dimethy1-5-sulfo- (CA INDEX NAME)
 C44 H47 N6 013 S2 CN
- MF
- CICOM
- SR CA

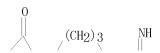
HO3S Me Me CH-CH=CH-CH=CH-CH=SO3H (CH2)
$$5$$
-C-NH-CH2-CH2-N

- ANSWER 6 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- 944336-77-0 REGISTRY Entered STN: 09 Aug 2007 ED
- $L-Cystein a mide, \ \ gly cyl-L-arginyl-L-lysyl-L-lysyl-L-arginy$ CNglutaminyl-L-arginyl-L-arginyl-L-arginylglycyl-S-[1-[2-[6-[2-[5-(3-ethyl-1, 3-dihydro-1, 1-dimethyl-6, 8-disulfo-2H-benz[e]indol-2-ylidene)-1, 3pentadien-1-yl]-1, 1-dimethyl-6, 8-disulfo-1H-benz[e]indolio]-1oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (CA INDEX
- FS PROTEIN SEQUENCE; STEREOSEARCH
- MF C107 H168 N38 028 S5
- SR CA
- STN Files: CA, CAPLUS LC

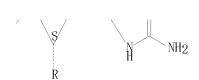
RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry. Double bond geometry unknown.

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1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 7 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- 918959-25-8 REGISTRY Entered STN: 01 Feb 2007 ED
- $L-Cystein a mide, \ N-acetyl-L-histidyl-L-$ CNhistidyl-L-histidylglycyl-L-leucyl-2-methylalanyl-L-alanyl-L-alanyl-L-alanylglycylglycyl-L-tryptophylglycyl-S-[1-[2-[[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1-propen-1-yl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (CA INDEX NAME)
- FS PROTEIN SEQUENCE; STEREOSEARCH
- MF C113 H146 N34 O26 S3
- SR CA
- LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry. Double bond geometry unknown.

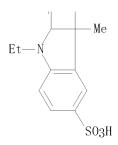
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1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 8 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 911318-70-2 REGISTRY
 Entered STN: 26 Oct 2006
 3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dioxo-1-pyrrolidinyl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-5-(2-thienyl)-2H-indol-2-ylidene]-1, 3-dihydro-3, 3-dimethyl-5-(3-thienyl)-2H-indol-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2H-indol-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2H-indol-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2H-indol-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2H-indol-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2H-indol-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2H-indol-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2-ylidene]-1, 3-dimethyl-5-(3-thienyl)-2-ylidene]-1, 3-dimethyl-3-dimethyl-5-(3-thienyl)-2-ylidene]-1, 3-dimethyl-3-di CNpentadien-1-yl]-1-ethyl-3, 3-dimethyl-5-nitro- (CA INDEX NAME)

OTHER CA INDEX NAMES:

- oxohexyl]-1, 3-dihydro-3, 3-dimethyl-5-(2-thienyl)-2H-indol-2-ylidene]-1, 3pentadienyl]-1-ethyl-3, 3-dimethyl-5-nitro- (9CI)
- MF C43 H50 N5 05 S
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 9 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- 848301-88-2 REGISTRY Entered STN: 12 Apr 2005 ED
- Guanosine 5'-(trihydrogen diphosphate), P'-anhydride with CN S-[1-[2-[[6-[2-[5-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1,3-pentadienyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl] dihydrogen phosphorothioate (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MFC49 H62 N9 O22 P3 S3
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

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- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 10 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- 795315-59-2 REGISTRY Entered STN: 09 Dec 2004 ED
- L-Cysteinamide, glycyl-L-seryl-L-methionyl-L-leucyl-L-prolyl-L-valyl-L-threonyl-L-leucylglycyl-S-[1-[2-[[6-[2-[5-(3-ethyl-1,3-dihydro-1,1-dimethyl-6,8-disulfo-2H-benz[e]indol-2-ylidene)-1,3-pentadienyl]-1,1-dimethyl-6,8-disulfo-1H-benz[e]indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CA INDEX NAME)
 PROTEIN SEQUENCE; STEREOSEARCH CN
- FS
- MFC88 H123 N15 027 S6
- SR CA
- STN Files: LC CA, CAPLUS

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1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 11 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 795315-58-1 REGISTRY
 Entered STN: 09 Dec 2004
 L-Cysteinamide, N-[[2-[2-[3-[[5-carboxy-1, 3-dihydro-3, 3-dimethyl-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-chloro-1-cyclohexen-1-CNyl]ethenyl]-3,3-dimethyl-1-(4-sulfobutyl)-3H-indolium-5-yl]carbonyl]glycyl-L-valyl-L-prolyl-L-leucyl-L-seryl-L-leucyl-L-threonyl-L-methionylglycyl-S-[1-[2-[6-[2-[5-(3-ethyl-1,3-dihydro-1,1-dimethyl-6,8-disulfo-2Hbenz[e]indol-2-ylidene)-1,3-pentadienyl]-1,1-dimethyl-6,8-disulfo-1Hbenz[e]indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, bis(inner salt) (9CI) (CA INDEX NAME)
- PROTEIN SEQUENCE; STEREOSEARCH FS
- MF C128 H168 C1 N17 036 S8
- SR CA
- LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry. Double bond geometry unknown.

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1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 12 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 756898-10-9 REGISTRY
 Entered STN: 05 Oct 2004
 Coenzyme A, S-[1-[2-[[6-[2-[5-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1,3-pentadienyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CA CN INDEX NAME)
- FS STEREOSEARCH
- DR 801306-66-1
- MF C60 H82 N11 025 P3 S3
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE) 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:382041 REFERENCE 2: 142:19000 REFERENCE 3: 141:256678

- ANSWER 13 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 756898-09-6 REGISTRY
 Entered STN: 05 Oct 2004
 Coenzyme A, S-[1-[2-[[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1-propenyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-CN oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) INDEX NAME)
- FS STEREOSEARCH
- DR 801306-65-0
- MF C58 H80 N11 O25 P3 S3
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE) 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:382041 REFERENCE 2: 142:19000 REFERENCE 3: 141:256678

- ANSWER 14 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644979-01-1 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1-CNpropen-1-y1]-1, 3, 3-trimethyl-5-sulfo-, inner salt (CA INDEX NAME) OTHER CA INDEX NAMES:
- 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1propenyl]-1, 3, 3-trimethyl-5-sulfo-, inner salt (9CI)
- FS STEREOSEARCH
- MF C36 H42 N4 06 S
- SR CA
- STN Files: LC CA, CAPLUS, USPATFULL

Double bond geometry as shown.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 15 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644979-00-0 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-CN1, 3-pentadien-1-yl]-3, 3-dimethyl-1-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

OTHER CA INDEX NAMES:

- 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadienyl]-3,3-dimethyl-1-(4-sulfobutyl)-, inner salt (9CI)
- FS STEREOSEARCH
- MF C41 H50 N4 O6 S
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1: 140:90327 REFERENCE

- ANSWER 16 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644978-99-4 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[3-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)propyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-CN1-propen-1-y1]-3, 3-dimethyl-1-(4-sulfobutyl)-, inner salt (CA INDEX NAME) OTHER CA INDEX NAMES:
- 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[3-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)propyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1-propeny1]-3, 3-dimethy1-1-(4-sulfobuty1)-, inner salt (9CI)
- FS STEREOSEARCH
- MF C40 H50 N4 06 S
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 17 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644978-98-3 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[3-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)propyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-CN1-propen-1-yl]-1-ethyl-3, 3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME) OTHER CA INDEX NAMES:
- 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[3-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)propyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1-propenyl]-1-ethyl-3, 3-dimethyl-5-sulfo-, inner salt (9CI)
- FS STEREOSEARCH
- MF C38 H46 N4 06 S
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1: 140:90327 REFERENCE

- ANSWER 18 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644978-97-2 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[5-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-5-oxopentyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-CN1, 3-pentadien-1-yl]-3, 3-dimethyl-1-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

OTHER CA INDEX NAMES:

- 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[5-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)ethyl]amino]-5-oxopentyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1, 3-pentadienyl]-3, 3-dimethyl-1-(4-sulfobutyl)-, inner salt (9CI)
- FS STEREOSEARCH
- MF C40 H48 N4 06 S
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 19 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644978-96-1 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1-CNpropen-1-yl]-3, 3-dimethyl-1-(4-sulfobutyl)-, inner salt (CA INDEX NAME) OTHER CA INDEX NAMES:
- 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1propenyl]-3, 3-dimethyl-1-(4-sulfobutyl)-, inner salt (9CI)
- FS STEREOSEARCH
- MF C39 H48 N4 06 S
- SR CA
- STN Files: LC CA, CAPLUS, USPATFULL

Double bond geometry as shown.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 20 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644978-95-0 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[5-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-5-oxopentyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-CN1, 3-pentadien-1-yl]-1-ethyl-3, 3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

OTHER CA INDEX NAMES:

- 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[5-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)ethyl]amino]-5-oxopentyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadienyl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (9CI)
- FS STEREOSEARCH
- MF C38 H44 N4 06 S
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 21 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644978-94-9 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-CN1, 3-pentadien-1-yl]-1-ethyl-3, 3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

OTHER CA INDEX NAMES:

- 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadienyl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (9CI)
- FS STEREOSEARCH
- MF C39 H46 N4 06 S
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 22 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644978-93-8 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1-CNpropen-1-yl]-3, 3-dimethyl-1-propyl-5-sulfo-, inner salt (CA INDEX NAME) OTHER CA INDEX NAMES:
- 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1propenyl]-3, 3-dimethyl-1-propyl-5-sulfo-, inner salt (9CI)
- FS STEREOSEARCH
- MF C38 H46 N4 06 S
- SR CA
- STN Files: LC CA, CAPLUS, USPATFULL

Double bond geometry as shown.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 23 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644978-92-7 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-CN1, 3-pentadien-1-yl]-1, 3, 3-trimethyl-5-sulfo-, inner salt (CA INDEX NAME) OTHER CA INDEX NAMES:
- 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadienyl]-1,3,3-trimethyl-5-sulfo-, inner salt (9CI)
- FS STEREOSEARCH
- MF C38 H44 N4 06 S
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:34835

- ANSWER 24 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 644978-91-6 REGISTRY
 Entered STN: 02 Feb 2004
 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1-CNpropen-1-yl]-1-ethyl-3, 3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME) OTHER CA INDEX NAMES:
- $3 \\ \\ \text{H-Indolium, } 2 \\ -[(1E, 3E) \\ \\ -3 \\ -[1 \\ -[6 \\ -[[2 \\ (2, 5 \\ \\ \\ \\ \text{dihydro-} 2, 5 \\ \\ \\ -\text{dioxo-} 1 \\ \\ \\ \\ \\ +\text{pyrrol-} 1 \\ \\ -\text{dioxo-} 1 \\ \\ \\ +\text{pyrrol-} 1 \\ \\ -\text{dioxo-} 1 \\ \\ +\text{dioxo-} 2 \\ \\ +\text{dioxo-} 1 \\ \\ +\text{dioxo-} 2 \\ \\ +\text{dioxo-}$ yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1propenyl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (9CI)
- FS STEREOSEARCH
- MF C37 H44 N4 06 S
- SR CA
- STN Files: LC CA, CAPLUS, USPATFULL

Double bond geometry as shown.

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:34835

REFERENCE 2: 140:90327

- ANSWER 25 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3
- RN
- ED
- 616207-80-8 REGISTRY
 Entered STN: 13 Nov 2003
 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohayyl]-1, 3-dihydro-3, 3-dimethyl-5-sulfo-2H-indol-2-CN ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

OTHER CA INDEX NAMES:

- 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2ylidene]-1-propenyl]-1-ethyl-3, 3-dimethyl-5-sulfo-, inner salt (9CI) OTHER NAMES:
- CN Cy3 Maleimide
- MF C37 H44 N4 O9 S2
- SR CA
- STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL LC

- 13 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 150:17227

REFERENCE 2: 149:4549

REFERENCE 3: 148:373658

REFERENCE 147:359757

REFERENCE 5: 146:312090

REFERENCE 145:371937

REFERENCE 145:119607 7:

REFERENCE 8: 144:116713

REFERENCE 144:57536

REFERENCE 10: 142:19000

ANSWER 26 OF 26 REGISTRY COPYRIGHT 2009 ACS on STN L3

RN

ED

416853-49-1 REGISTRY
Entered STN: 16 May 2002
3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-y1)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1, 3-pentadien-1-yl]-1-ethyl-3, 3-dimethyl-5-sulfo-, inner salt CN(CA INDEX NAME)

OTHER CA INDEX NAMES:

3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-5-sulfo-2H-indol-2ylidene]-1,3-pentadienyl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (9CI)

C39 H46 N4 09 S2 MF

SR

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

HO3S Me Me CH-CH-CH-CH-CH-CH-
$$^{\rm CH}$$
 Me Me S03-

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1: 142:19000 REFERENCE

REFERENCE 141:256678 2:

REFERENCE 3: 136:337160 => fil capl FILE 'CAPLUS' ENTERED AT 14:23:44 ON 08 JAN 2009 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

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http://www.cas.org/legal/infopolicy.html '.FIONA' IS DEFAULT FORMAT FOR 'CAPLUS' FILE

=> s 13 L4 25 L3

=> d 1-25 bib abs hitstr

- L4 ANSWER 1 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2008:1343832 CAPLUS
- DN 150:17227
- TI LCP-FRAP Assay for Pre-Screening Membrane Proteins for In Meso Crystallization
- AU Cherezov, Vadim; Liu, Jeffrey; Griffith, Mark; Hanson, Michael A.; Stevens, Raymond C.
- CS Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
- SO Crystal Growth & Design (2008), 8(12), 4307-4315 CODEN: CGDEFU; ISSN: 1528-7483
- PB American Chemical Society
- DT Journal
- LA English
- Fluorescence recovery after photobleaching was used to study the diffusion AB of two integral membrane proteins, bacteriorhodopsin and beta2-adrenergic receptor, in lipidic cubic phase (LCP). The authors found that the diffusion properties within the LCP matrix strongly depend on the protein construct and applied screening conditions. Common precipitants often induce restriction on diffusion of proteins in LCP and thereby impede their chances for crystallization A high protein mobile fraction and a fast diffusion rate correlate well with known crystallization conditions. Using this knowledge, one can now prescreen precipitant conditions with microgram quantities of material to rule out conditions that are not conducive to diffusion, nucleation, and crystal growth. The results of this assay will narrow membrane protein crystallization space by identifying suitable protein constructs, stabilizing compds. and precipitant conditions amenable to in meso crystallization Crystallization prescreening will significantly increase the chances of obtaining initial crystal hits, expediting efforts in generating high-resolution structures of challenging membrane protein targets. ΙT 616207-80-8
- RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
 - (lipidic cubic phase-fluorescence recovery after photobleaching assay for pre-screening membrane proteins for in meso crystallization)
- RN 616207-80-8 CAPLUS
- CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-y1)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2008:1150206 CAPLUS
- DN 149:464926
- TI Modified Peptides as Potent Inhibitors of the Postsynaptic Density-95/N-Methyl-D-Aspartate Receptor Interaction
- AU Bach, Anders; Chi, Celestine N.; Olsen, Thomas B.; Pedersen, Soren W.; Roder, Martin U.; Pang, Gar F.; Clausen, Rasmus P.; Jemth, Per; Stromgaard, Kristian
- CS Department of Medicinal Chemistry, The Faculty of Pharmaceutical Sciences, University of Copenhagen, Copenhagen, DK-2100, Den.
- SO Journal of Medicinal Chemistry (2008), 51(20), 6450-6459 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
- LA English
- AR The protein-protein interaction between the NMDA receptor and its intracellular scaffolding protein, PSD-95, is a potential target for treatment of ischemic brain diseases. An undecapeptide corresponding to the C-terminal of the NMDA was used as a template for finding lead candidates for the inhibition of the PSD-95/NMDA receptor interaction. Initially, truncation and alanine scan studies were carried out, which resulted in a pentapeptide with wild-type affinity, as examined in a fluorescence polarization assay. Further examination was performed by systematic substitutions with natural and unnatural amino acids, which disclosed a tripeptide with micromolar affinity and N-methylated tetrapeptides with improved affinities. Mol. modeling studies guided further N-terminal modifications and introduction of a range of N-terminal substitutions dramatically improved affinity. The best compound, N-cyclohexylethyl-ETAV (56), demonstrated up to 19-fold lower Ki value (Ki = 0.94 and 0.45 μ M against PDZ1 and PDZ2 of PSD-95, resp.) compared to wild-type values, providing the most potent inhibitors of this interaction reported so far. These novel and potent inhibitors provide an important basis for development of small mol. inhibitors of the PSD-95/NMDA receptor interaction.
- IT 1071969-30-6P 1071969-32-8P
 - RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 - (preparation of modified peptides for inhibition of postsynaptic d.-95/N-Me-D-aspartate receptor interaction)
- RN 1071969-30-6 CAPLUS
- CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-A

PAGE 1-B

PAGE 2-A

PAGE 2-B

RN 1071969-32-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 2-A

RE. CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2008:480760 CAPLUS
- DN 149:4549
- TI Measurement of Protein Sulfhydryls in Response to Cellular Oxidative Stress Using Gel Electrophoresis and Multiplexed Fluorescent Imaging Analysis
- AU Spiess, Page C.; Morin, Dexter; Jewell, William T.; Buckpitt, Alan R. CS Department of Molecular Biosciences, School of Veterinary Medicine,
 - University of California, Davis, CA, USA
- SO Chemical Research in Toxicology (2008), 21(5), 1074-1085 CODEN: CRTOEC; ISSN: 0893-228X
- PB American Chemical Society
- DT Journal
- LA English
- The significance of free radicals in biol. has been established by AB numerous investigations spanning a period of over 40 years. Whereas there are many intracellular targets for these radical species, the importance of cysteine thiol posttranslational modification has received considerable attention. The current studies present a highly sensitive method for measurement of the posttranslational modification of protein thiols. This method is based on labeling of proteins with monofunctional maleimide dyes followed by 2D gel electrophoresis to sep. proteins and multiplexed fluorescent imaging anal. The method correctly interrogates the thiol/disulfide ratio present in com. available proteins. Exposure of pulmonary airway epithelial cells to high concns. of menadione or t-Bu hydroperoxide resulted in the modification of cysteines in more than 141 proteins of which 60 were subsequently identified by MALDI-TOF/TOF MS. Although some proteins were modified similarly by these two oxidants, several showed detectably different maleimide ratios in response to these two agents. Proteins that were modified by one or both oxidants include those involved in transcription, protein synthesis and folding, and cell death/growth. In conclusion, these studies provide a novel procedure for measuring the redox status of cysteine thiols on individual proteins with a clearly demonstrated applicability to interactions of chems. with pulmonary epithelial cells.
- IT 616207-80-8
 - RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
 - (Cy3 maleimide; measurement of protein sulfhydryls in response to cellular oxidative stress using gel electrophoresis and multiplexed fluorescent imaging anal.)
- RN 616207-80-8 CAPLUS
- CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- 2008:378147 CAPLUS AN
- DN 148:373658
- ΤI Selective fluorescent labeling of S-nitrosothiols (S-FLOS): a novel method for studying S-nitrosylation
- IN Cole, Robert N.; Berkowitz, Dan E.; Santhanam, Lakshmi; Shoukas, Artin
- PA Johns Hopkins University, USA
- S0 PCT Int. Appl., 32pp. CODEN: PIXXD2
- DT
- Patent English
- LA

FAN. CNT 1 PATENT NO.					KIND		DATE		APPLICATION NO.					DATE			
PΙ	WO 2008	WO 2008036328			A2 20080327			WO 2007-US20328									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,	CA,
		CH,	CN,	СО,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,	FΙ,
		GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,
		KM,	KN,	KP,	KR,	KZ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,	ME,
		MG,	MK,	MN,	MW,	MX,	MY,	ΜZ,	NA,	NG,	ΝI,	ΝΟ,	NZ,	OM,	PG,	PH,	PL,
		PΤ,	RO,	RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	TJ,	TM,	TN,
		TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW				
	RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	IE,
		IS,	ΙT,	LT,	LU,	LV,	MC,	ΜT,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG,	BW,
		GH,	GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,
			,	,	MD,		TJ,	TM									
PRA]	[US 200€	8459	944P		Р		2006	0920									

A method and kit are described for selectively labeling S-nitrosylated cysteines in proteins with a fluorescent tag. The method offers femtomolar sensitivity for the detection, quantification, in situ visualization, and a means for site-specific identification of S-nitrosylation events. Proteins were incubated with 20 mM Me methanethiosulfonate at 50° to block free cysteines, reduced with buffer containing ascorbate, and labeled with Cy3- or Cy5-maleimide. ΙT 616207-80-8

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); RCT (Reactant); ANST (Analytical study); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(Cy3 maleimide; selective fluorescent labeling of S-nitrosylated cysteines in proteins with fluorescent tags)

RN

616207-80-8 CAPLUS 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-CN yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

- L4 ANSWER 5 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:805622 CAPLUS
- DN 147:359757
- TI Detection of Reactive Oxygen Species—sensitive Thiol Proteins by Redox Difference Gel Electrophoresis: implications for mitochondrial redox signaling
- AU Hurd, Thomas R.; Prime, Tracy A.; Harbour, Michael E.; Lilley, Kathryn S.; Murphy, Michael P.
- CS Medical Research Council Dunn Human Nutrition Unit, Cambridge, CB2 OXY, UK
- SO Journal of Biological Chemistry (2007), 282(30), 22040-22051 CODEN: JBCHA3; ISSN: 0021-9258
- PB American Society for Biochemistry and Molecular Biology
- DT Iournal
- LA English
- Reactive oxygen species (ROS) produced by the mitochondrial respiratory AB chain can be a redox signal, but whether they affect mitochondrial function is unclear. Here the authors show that low levels of ROS from the respiratory chain under physiol, conditions reversibly modify the thiol redox state of mitochondrial proteins involved in fatty acid and carbohydrate metabolism As these thiol modifications were specific and occurred without bulk thiol changes, the authors first had to develop a sensitive technique to identify the small number of proteins modified by endogenous ROS. In this technique, redox difference gel electrophoresis, control, and redox-challenged samples are labeled with different thiol-reactive fluorescent tags and then separated on the same two-dimensional gel, enabling the sensitive detection of thiol redox modifications by changes in the relative fluorescence of the two tags within a single protein spot, followed by protein identification by mass spectrometry. Thiol redox modification affected enzyme activity, suggesting that the reversible modification of enzyme activity by ROS from the respiratory chain may be an important and unexplored mode of mitochondrial redox signaling.
- IT 616207-80-8

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(Cy3 Maleimide, labeling; detection of reactive oxygen species-sensitive thiol proteins by redox difference gel

electrophoresis and implications for mitochondrial redox signaling)

RN 616207-80-8 CAPLUS

CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:520264 CAPLUS
- DN 147:186998
- TI In vivo monitoring the fate of Cy5.5-Tat labeled T lymphocytes by quantitative near-infrared fluorescence imaging during acute brain inflammation in a rat model of experimental autoimmune encephalomyelitis
- AU Berger, Cedric; Gremlich, Hans-Ulrich; Schmidt, Philipp; Cannet, Catherine; Kneuer, Rainer; Hiestand, Peter; Rausch, Martin; Rudin, Markus
- CS Novartis Institutes for Biomedical Research, Basel, Switz.
- SO Journal of Immunological Methods (2007), 323(1), 65-77 CODEN: JIMMBG; ISSN: 0022-1759
- PB Elsevier B.V.
- DT Journal
- LA English
- AB T cells and macrophages directed against myelin proteins orchestrate the inflammation process in multiple sclerosis (MS) and exptl. autoimmune encephalomyelitis (EAE). So far, assessment of macrophages infiltration or structural alterations has been achieved by in vivo imaging. work, the authors show the infiltration of Cy5.5-labeled T lymphocytes into the brains of EAE rats by reflectance near-IR fluorescence imaging. T lymphocytes were labeled with Cy5.5-Tat and administered i.v. to naive or EAE animals. The highest fluorescence signal was observed for EAE animals, which received myelin-activated T cells during the acute phase of the disease. The temporal profile of fluorescence in this group paralleled the pattern of neurol. impairment during the acute phase, the remittance and first relapses of EAE. No disease specific fluorescence pattern was observed for EAE animals, which received naive T cells. However, uptake of Cy5.5-Tat by scavenger cells (e.g. macrophages) following death of labeled T cells in vivo prevents prolonged longitudinal studies. This work demonstrates that Cy5.5-Tat labeling of T cells is suitable for in vivo fluorescence imaging of inflammation initiation in the EAE model. This approach may particularly be useful for evaluation of novel anti-inflammatory therapies.
- IT 944336-77-0
 - RL: BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
 - (near-IR fluorescence imaging of T-cell infiltration in multiple sclerosis model using Cy5.5-Tat)
- RN 944336-77-0 CAPLUS
- CN L-Cysteinamide, glycyl-L-arginyl-L-lysyl-L-arginyl-L-arginyl-L-glutaminyl-L-arginyl-L-arginyl-L-arginylglycyl-S-[1-[2-[[6-[2-[5-(3-ethyl-1,3-dihydro-1,1-dimethyl-6,8-disulfo-2H-benz[e]indol-2-ylidene)-1,3-pentadien-1-yl]-1,1-dimethyl-6,8-disulfo-1H-benz[e]indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-B

PAGE 2-B

PAGE 3-B

RE. CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:347882 CAPLUS
- DN 147:253147
- TI Construction of Ni2+ion responding type block coiled coil and application for new sensing material
- AU Kashiwada, Ayumi; Matsuda, Kiyomi
- CS Dep. of Production Engineering, Nihon Univ., Japan
- SO Nihon Daigaku Seisan Kogakubu Haiteku Risachi Senta Kenkyu Hokokusho (2006), Volume Date 2005 25-28
 CODEN: NDSKCG
- PB Nihon Daigaku Seisan Kogakubu Seisan Kogaku Kenkyusho
- DT Journal
- LA Japanese
- AB Hetero-block peptide α-helical coiled coil formation with Ni2+ ion and application of the block type complex sensoring module were reported. Formations of coiled coil conformation of specific peptides (Pep3 and Pep4) with Ni2+ were speculated by CD spectra. Metal-binding affinity of the structure was found to be more specific to Ni2+ than Cu2+ and Zn2+. The Ni2+-sensing system using other peptides (Pep5 and Pep6) was applied to fabrication of sensing system using Cy3B-Cy5Q FRET anal. was also reported.
- IT 945985-10-4D, Cy 5Q, conjugates with peptides
 - RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (Cy 5Q; construction of Ni2+ion responding type block coiled coil and application for new sensing material)
- RN 945985-10-4 CAPLUS
- CN 3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-1-[(3,5-dinitrophenyl)methyl]-3,3-dimethyl-5-sulfo-,2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 945985-09-1 CMF C44 H47 N6 013 S2

CM 2

CRN 14477-72-6 CMF C2 F3 O2

- L4 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:195232 CAPLUS
- DN 147:400216
- TI Probing orientations of single fluorescent labels on a peptide reversibly binding to the human delta-opioid receptor
- AU Tokimoto, Takahira; Bethea, Tomika R. C.; Zhou, Min; Ghosh, Indraneel; Wirth, Mary J.
- CS Department of Chemistry, University of Arizona, Tucson, AZ, 85721, USA
- SO Applied Spectroscopy (2007), 61(2), 130-137 CODEN: APSPA4; ISSN: 0003-7028
- PB Society for Applied Spectroscopy
- DT Journal
- LA English
- We report the first in-depth study of single-mol. polarization behavior of AB a species that is undergoing reversible binding with its biol. receptor. We examine the utility of the information in single-mol. polarization measurements for investigations of binding. The human δ -opioid receptor, which is a G protein-coupled receptor, was incorporated into a supported lipid bilayer. A Cy3 label was covalently attached by a hydrophilic linker to a peptide agonist, Deltorphin II (5,6 Ile-Ile). The fluorescence excitation was alternated between s- and p-polarization using a microscope having the capability of total internal reflectance fluorescence (TIRF) excitation. The polarization behavior reveals that nonspecific binding events for this system give emission that is mostly s-polarized, while binding to the receptor gives emission that has a strong component of p-polarization. The results show that a high signal-to-noise ratio is achievable with single-mol. polarization measurements. The experiment detected 37 binding events of short duration (<30 s) and 35 binding events of long duration (from 30 s to 500 s). The polarization studies indicate that the receptors in the bilayer do not freely rotationally diffuse in the plane of the bilayer when the peptide is bound. The system exhibits two types of polarization behavior. One type has the dye label with fixed orientation, which sometimes abruptly switches. The other type has the dye orientation continuously fluctuating over time, typically exhibiting occasional periods of fixed orientation. For a long binding event of fixed orientation, it is established through anal. of the variance that the orientation actually is fluctuating through a range of angles on the order of 6° . It is shown that precise measurements of reorientation are achievable, with a detection limit of 1.3° for a typical single-mol. signal.
- IT 950890-22-9
 - RL: BSU (Biological study, unclassified); BIOL (Biological study) (orientations of single fluorescent labels on a peptide reversibly binding to the human delta-opioid receptor)
- RN 950890-22-9 CAPLUS
- CN Glycinamide, L-tyrosyl-D-alanyl-L-phenylalanyl-L- α -glutamyl-L-isoleucyl-L-isoleucylglycylglycyl-18-amino-5-oxo-3, 9, 12, 15-tetraoxa-6-azaoctadecanoyl-S-[1-[2-[[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1-propen-1-yl]-3, 3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2, 5-dioxo-3-pyrrolidinyl]-L-cysteinyl-, inner salt (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

H03S Me Me Me S03
$$^-$$
 S03 $^-$ Et (CH2)5 0 0 S R

PAGE 1-B

PAGE 1-C

PAGE 1-D

RE. CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:51214 CAPLUS
- DN 146:312090
- TI Site-specific labeling of DNA-protein conjugates by means of expressed protein ligation
- AU Lovrinovic, Marina; Fruk, Ljiljana; Schroeder, Hendrik; Niemeyer, Christof M.
- CS Fachbereich Chemie, Biologisch-Chemische Mikrostrukturtechnik, Universitaet Dortmund, Dortmund, D-44227, Germany
- SO Chemical Communications (Cambridge, United Kingdom) (2007), (4), 353-355 CODEN: CHCOFS; ISSN: 1359-7345
- PB Royal Society of Chemistry
- DT Journal
- LA English
- AB Site-specific bioconjugation of protein thioesters with a DNA oligonucleotide was achieved by Expressed Protein Ligation (EPL) and the new thiol group formed upon EPL in the conjugate was selectively coupled with small mol. labels using maleimide chemical
- IT 616207-80-8, Cy3 Maleimide
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST
 (Analytical study); BIOL (Biological study); USES (Uses)
 (Cy3 Maleimide; site-specific labeling of DNA-protein conjugates by
 means of expressed protein ligation)
- RN 616207-80-8 CAPLUS
- CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

Ι

- L4 ANSWER 10 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- 2006:1041247 CAPLUS AN
- DN 145:392008
- ΤI Chemically-reactive cyanine dyes and their applications as luminescence quenching compounds
- Diwu, Zhenjun; Zhang, Jianheng; Tang, Yi ΤN
- PA Anaspec, Inc., USA
- S0 U.S. Pat. Appl. Publ., 40pp. CODEN: USXXCO
- DΤ Patent
- English LA

FAN. CNT 1				
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 20060223076 PRAI US 2004-608817P	A1 P	20061005 20040910	US 2005-222049	20050907
OS MARPAT 145:392008				
GI				

$$\begin{array}{c|c} & \text{Me Me} \\ & \text{Me} \\ & \text{N}^+ \\ & & \text{C02}^- \\ & \text{II} \end{array}$$

- The quenching compds. of the invention are weakly luminescent cyanines AB that are substituted by one or more heteroarom, quenching moieties. quenching compds. of the invention exhibit little or no observable luminescence and efficiently quench a broad spectrum of luminescent The chemical reactive quenching compds. possess utility for labeling a wide variety of substances, including biomols. These labeled substances are highly useful for a variety of energy-transfer assays and applications. Reactive quenching cyanine dye I was prepared from II, malonaldehyde bis(phenylimine) monohydrochloride, and 1,3-diethyl-2-methylimidazolium iodide. The FRET peptide, compound I-Lys-Pro-Leu-Ala-Nva-Asp(Cy5)-Ala-Arg-NH2, was incubated with solns. with or without matrix metalloproteinase 2 and the fluorescence signal was recorded on a fluorescence microplate reader at Ex/Em=650nm/670nm. 911318-70-2P ΙT
 - RL: SPN (Synthetic preparation); PREP (Preparation) (chemical-reactive cyanine dyes and their applications as luminescence quenching compds.)
- RN
- 911318-70-2 CAPLUS 3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dioxo-1-pyrrolidinyl)ethyl]amino]-6-CN oxohexyl]-1, 3-dihydro-3, 3-dimethyl-5-(2-thienyl)-2H-indol-2-ylidene]-1, 3pentadien-1-yl]-1-ethyl-3, 3-dimethyl-5-nitro- (CA INDEX NAME)

- L4 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2006:799922 CAPLUS
- DN 145:371937
- TI Binding and signaling of surface-immobilized reagentless fluorescent biosensors derived from periplasmic binding proteins
- AU De Lorimier, Robert M.; Tian, Yaji; Hellinga, Homme W.
- CS Department of Biochemistry, Duke University Medical Center, Durham, NC, 27710, USA
- SO Protein Science (2006), 15(8), 1936-1944
 - CODEN: PRCIEI; ISSN: 0961-8368
- PB Cold Spring Harbor Laboratory Press
- DT Journal
- LA English
- AB Development of biosensor devices typically requires incorporation of the mol. recognition element into a solid surface for interfacing with a signal detector. One approach is to immobilize the signal transducing protein directly on a solid surface. Here the authors compare the effects of two direct immobilization methods on ligand binding, kinetics, and signal transduction of reagentless fluorescent biosensors based on engineered periplasmic binding proteins. The authors used thermostable ribose and glucose binding proteins cloned from Thermoanaerobacter tengcongensis and Thermotoga maritima, resp. To test the behavior of these proteins in semispecifically oriented layers, the authors covalently modified lysine residues with biotin or sulfhydryl functions, and attached the conjugates to plastic surfaces derivatized with streptavidin or maleimide, resp. The immobilized proteins retained ligand binding and signal transduction but with adversely affected affinities and signal amplitudes for the thiolated, but not the biotinylated, proteins. The authors also immobilized these proteins in a more specifically oriented layer to maleimide-derivatized plates using a His2Cys2 zinc finger domain fused at either their N or C termini. Proteins immobilized this way either retained, or displayed enhanced, ligand affinity and signal amplitude. In all cases tested ligand binding by immobilized proteins is reversible, as demonstrated by several iterations of ligand loading and elution. The kinetics of ligand exchange with the immobilized proteins are on the order of seconds.
- IT 616207-80-8D, Cy3 Maleimide, ligand-binding protein conjugates RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); DEV (Device component use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
 - (Cy3-maleimide; binding and signaling of surface-immobilized reagentless fluorescent biosensors derived from periplasmic binding proteins)
- RN 616207-80-8 CAPLUS
- CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2006:458964 CAPLUS
- DN 145:119607
- TI Designer Variable Repeat Length Polypeptides as Scaffolds for Surface Immobilization of Quantum Dots
- AU Medintz, Igor L.; Sapsford, Kim E.; Clapp, Aaron R.; Pons, Thomas; Higashiya, Seiichiro; Welch, John T.; Mattoussi, Hedi
- CS Center for Bio/Molecular Science and Engineering, Code 6900, U.S. Naval Research Laboratory, Washington, DC, 20375, USA
- SO Journal of Physical Chemistry B (2006), 110(22), 10683-10690 CODEN: JPCBFK; ISSN: 1520-6106
- PB American Chemical Society
- DT Journal
- LA English
- The authors demonstrate the use of a series of engineered, variable-length AB de novo polypeptides to discretely immobilize luminescent semiconductor nanocrystals or quantum dots (QDs) onto functional surfaces. polypeptides express N-terminal dicysteine and C-terminal hexahistidine residues that flank a variable number (1, 3, 5, 7, 14, 21, 28, or 35) of core β -strand repeats, with tyrosine, glutamic acid, histidine, and lysine residues located at the turns. Polypeptides have mol. wts. ranging from 4 to 83 kDa and retain a rigid structure based on the antiparallel β -sheet motif. The authors first use a series of dye-labeled polypeptides to test and characterize their self-assembly onto hydrophilic CdSe-ZnS QDs using fluorescence resonance energy transfer (FRET). Results indicate that peptides maintain their β -sheet conformation after self-assembly onto the QD surfaces, regardless of their length. authors then immobilize biotinylated derivs. of these polypeptides on a NeutrAvidin-functionalized substrate and use them to capture QDs via specific interactions between the peptides' polyhistidine residues and the nanocrystal surface. The authors found that each of the polypeptides was able to efficiently capture QDs, with a clear correlation between the d. of the surface-tethered peptide and the capacity for nanocrystal capture. The versatility of this capture strategy is highlighted by the creation of a variety of one- and two-dimensional polypeptide-QD structures as well as a self-assembled surface-immobilized FRET-based nutrient sensor.
- IT 616207-80-8D, Cy3 maleimide, maltose binding protein conjugates RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); DEV (Device component use); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(designer variable repeat length polypeptides as scaffolds for surface immobilization of quantum dots and application to maltose FRET-based sensor)

- RN 616207-80-8 CAPLUS
- CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2006:401255 CAPLUS
- DN 146:137336
- TI Quantum-dot-based nanosensors designed for proteolytic monitoring
- AU Medintz, Igor L.; Clapp, Aaron R.; Brunel, Florence M.; Goldman, Ellen R.; Chang, Eddie L.; Dawson, Phillip E.; Mattoussi, Hedi
- CS US Naval Research Lab., Center for Bio/Molecular Science and Engineering, Washington, DC, 20375, USA
- SO Proceedings of SPIE-The International Society for Optical Engineering (2006), 6096(Colloidal Quantum Dots for Biomedical Applications), 60960K/1-60960K/8
 CODEN: PSISDG; ISSN: 0277-786X
- PB SPIE-The International Society for Optical Engineering
- DT Journal
- LA English
- AB The authors have previously assembled QD-based fluorescence resonance energy transfer (FRET) sensors specific for the sugar nutrient maltose and the explosive TNT. These sensors utilize several inherent benefits of QDs as FRET donors. The authors show that QD-FRET based sensors can also function in the monitoring of proteolytic enzyme activity. The authors utilize a QD with multiple dye-labeled proteins attached to the surface as a substrate for a prototypical protease. The authors then demonstrate how this strategy can be extended to detect protease activity by utilizing a dye-labeled peptide attached to the QD as a proteolytic substrate. Self-assembly of the peptide-dye on the QD brings the dye in close proximity to the QD and result in efficient FRET. Addition of a proteolytic enzyme that specifically recognizes and cleaves the peptide alters the FRET signature of the sensor in a concentration-dependent manner. Both qual. and quant. data can be derived from these sensors. The potential benefits of this type of QD sensing strategy are discussed. ΙT 918959-25-8P
 - RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)

(quantum-dot-based fluorescence resonance energy transfer nanosensors designed for proteolytic enzyme monitoring)

RN 918959-25-8 CAPLUS

CN L-Cysteinamide, N-acetyl-L-histidyl-L-histidyl-L-histidyl-L-histidyl-L-histidyl-L-histidyl-L-histidyl-L-histidyl-L-histidyl-L-alanyl-L-alanyl-L-alanylglycyl-L-tryptophylglycyl-S-[1-[2-[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1-propen-1-yl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 1-D

PAGE 2-A

RE. CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
    ANSWER 14 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
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AN 2005:1314108 CAPLUS

DN 144:57536

ΤI Unagglomerated core/shell nanocomposite particles for biomedical applications

Adair, James H.; Rouse, Sarah M.; Wang, Jun; Kester, Mark; Siedlecki, IN Christopher; White, William B.; Vogler, Erwin; Snyder, Alan; Pantano, Carlo G.; Sinoway, Lawrence; Luck, Jerry

PA The Penn State Research Foundation, USA; Ruiz-Velasco, Victor

S0 PCT Int. Appl., 71 pp., which

CODEN: PIXXD2

DT Patent

LA English

FAN.	CNT	1
	PA'	ΓENT

	PA'	PATENT NO.					KIND DATE			APPLICATION NO.						DATE		
PΙ) 2005118702) 2005118702				A2 A3		20051215 20071115		WO 2005-US19239					20050601			
		W:	AE, CN, GE, LC,	AG, CO, GH, LK, NI,	AL, CR, GM, LR, NO,	AM, CU, HR, LS, NZ,	AT, CZ, HU, LT, OM,	AU, DE, ID, LU, PG, TN,	AZ, DK, IL, LV, PH,	DM, IN, MA, PL,	DZ, IS, MD, PT,	EC, JP, MG, RO,	EE, KE, MK, RU,	EG, KG, MN, SC,	ES, KM, MW, SD,	FI, KP, MX, SE,	GB, KR, MZ, SG,	GD, KZ, NA, SK,
		RW:	BW, AZ, EE, RO,	GH, BY, ES, SE,	GM, KG, FI, SI,	KZ, FR, SK,	MD, GB, TR,	MW, RU, GR, BF,	TJ, HU, BJ,	TM, IE, CF,	AT, IS, CG,	BE, IT,	BG, LT,	CH, LU,	CY, MC,	CZ, NL,	DE, PL,	DK, PT,
	AU 2005250464																	
		CA 2569067 US 20050281884								CA 2005-2569067 US 2005-142913								
	EΡ	1773	936			A2		2007	0418	EP 2005-804865						20050601		
		R:	IS,	IT,	LI,	LT,		CZ, MC,										
	TP	HR, LV, MK,		Т	20080124			JP 2007-515527					20050601					
		JP 2008501509 IN 2006KN03632				Ā				IN 2006-KN3632					20050001			
		KR 2007028478			A	20070312			KR 2006-727906					20061229				
PRAI	US	JS 2004-575887P			Р		2004	0601										
		2004 2005				P W		$2004 \\ 2005$										

The present invention provides a method for the synthesis of AB unagglomerated, highly dispersed, stable core/shell nanocomposite particles comprised of preparing a reverse micelle microemulsion that contains nanocomposite particles, treating the microemulsion with a silane coupling agent, breaking the microemulsion to form a suspension of the nanocomposite particles by adding an acid/alc. solution to the microemulsion that maintains the suspension of nanocomposite particles at a pH of between about 6 and 7, and simultaneously washing and dispersing the suspension of nanocomposite particles, preferably with a size exclusion HPLC system modified to ensure unagglomeration of the nanocomposite particles. The primary particle size of the nanocomposite particles can range in diameter from between about 1 to 100 nm, preferably from between about 10 to 50 nm, more preferably about 10 to 20 nm, and most preferably about 20 nm. An example is given for synthesis and dispersion of Ag/SiO2 nanocomposite particles using HPLC compared to four conventional techniques.

616207-80-8, Cy3 Maleimide

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(unagglomerated core/shell nanocomposite particles for biomedical applications)

RN 616207-80-8 CAPLUS CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

- L4 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2005:921213 CAPLUS
- DN 143:382041
- TI Multicolor Imaging of Cell Surface Proteins
- AU Vivero-Pol, Laura; George, Nathalie; Krumm, Holger; Johnsson, Kai; Johnsson, Nils
- CS Institute of Chemical Sciences and Engineering, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, CH-1015, Switz.
- SO Journal of the American Chemical Society (2005), 127(37), 12770-12771 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 143:382041
- AB The authors report on a method for the multicolor imaging of cell surface proteins which is based on the labeling of carrier protein (CP) fusion proteins with different fluorophores. In one application, different generations of a cell surface protein can be sequentially labeled to discriminate between old and newly made copies. In another application, fusions to different CPs can be selectively labeled with different fluorophores in one sample. Both applications open up new ways for studying the properties of cell surface proteins of living cells.
- IT 756898-09-6 756898-10-9
 - RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
 - (multicolor imaging of cell surface proteins using fluorophore-labeled carrier protein-containing fusion proteins)
- RN 756898-09-6 CAPLUS
- CN Coenzyme A, S-[1-[2-[[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1-propenyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-B

RN

756898-10-9 CAPLUS Coenzyme A, S-[1-[2-[[6-[2-[5-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1,3-pentadienyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CA TYPEN MARC) CNINDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

PAGE 1-B

RE. CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2005:452002 CAPLUS
- DN 144:116713
- TI Effect of bin time on the photon counting histogram for one-photon excitation
- AU Perroud, Thomas D.; Huang, Bo; Zare, Richard N.
- CS Department of Chemistry, Stanford University, Stanford, CA, 94305-5080,
- SO ChemPhysChem (2005), 6(5), 905-912 CODEN: CPCHFT; ISSN: 1439-4235
- PB Wiley-VCH Verlag GmbH & Co. KGaA
- DT Journal
- LA English
- Photon counting histogram (PCH) model with the correction for 1-photon AB excitation is valid at multiple bin times. The fitted apparent brightness and concentration follow the 3-dimensional diffusion model. More importantly, the semi-empirical parameter, F, introduced in the PCH model for 1-photon excitation to correct for the non-Gaussian shape of the observation volume, shows small variations with different bin times. These variations are consistent with the phys. interpretation of F, and they do not affect the resolving power of the PCH model for 1-photon excitation. Based on these findings, the authors extend the time-independent PCH anal. to time-dependent photon counting multiple histograms (PCMH). considers the effect of bin time on the PCH parameters in a way that is similar to fluorescence intensity multiple distribution anal. (FIMDA). From the same set of data, PCMH exts. time-dependent parameters (diffusion time and triplet-state relaxation time) as well as time-independent parameters (true specific brightness and true average number of mols.). 3-4-fold exptl. difference in mol. brightness, PCMH can resolve each species in a 2-species sample and extract their resp. diffusion times even when fluorescence correlation spectroscopy cannot.
- IT 616207-80-8, Cy3 maleimide
 - RL: PRP (Properties)

(effect of bin time on photon counting histogram for one-photon excitation for)

- RN 616207-80-8 CAPLUS
- CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- 2005:284030 CAPLUS AN
- DN 142:330269
- ΤI Assay solution compositions and methods in high throughput screening for effectors of G protein-coupled receptors
- Fang, Ye; Ferrie, Ann M.; Hong, Yulong; Pai, Sadashiva K.; Peng, Jinlin; IN Webb, Brian L.
- PA USA
- U.S. Pat. Appl. Publ., 16 pp. S0 CODEN: USXXCO
- DT Patent
- LA English

FAN. CNT 1

PATENT NO.	. К	KIND DA	ATE A	PPLICATION	NO.	DATE
PI US 2005000	39953	A1 20	0050331 U	IS 2003-676	351	20030930
US 200601	48006	A1 20	0060706 U	IS 2005-312	776	20051221
PRAI US 2003-6	76351	B1 20	0030930			
AD DCC 1	7	C	· · · · · · · · · · · · · · · · · · ·	1 1 . 1 .		1

- Buffered assay solns. for performing either binding or functional assays on arrays G protein-coupled receptors, and methods for their use are described. The standardized buffer solution can be used in high throughput screening of G protein-coupled receptor arrays for effector ligands. The buffered assay solution has an underlying composition having: a buffer reagent with a pH in the range of about 6.5 to about 7.9; an inorg. salt of a monovalent or divalent cation, at a concentration from about 1 mM to about 500 mM; and optionally a combination of: a blocker reagent at a concentration of about 0.01 weight % to about 2 weight % of the composition, or a protease-inhibitor at a concentration of about 0.001 mM to about 100 mM. In an embodiment for functional assay uses, the composition is modified to also include a GTP-analog, a GDP salt, and an anti-oxidant.
- ΙT 848301-88-2D, analogs
 - RL: ARU (Analytical role, unclassified); ANST (Analytical study) (in assay medium; assay solution compns. and methods in high throughput screening for effectors of G protein-coupled receptors)
- RN
- 848301-88-2 CAPLUS Guanosine 5'-(trihydrogen diphosphate), P'-anhydride with S-[1-[2-[6-[2-[5-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-]]ylidene)-1, 3-pentadienyl]-3, 3-dimethyl-5-sulfo-3H-indolio]-1oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl] dihydrogen phosphorothioate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

$$-\mathrm{Et}$$
 Me Me $\mathrm{S03}^ \mathrm{(CH2)}\,\mathrm{5}$

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L4
     ANSWER 18 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
     2004:1059603 CAPLUS
AN
DN
     142:34835
     Differential analysis of cell surface proteins on closed membrane
ΤI
     structures by labelling with dyes in the presence of an internal standard
     Copse, Catherine; Fowler, Susan Janet; Horsey, Imogen; Sweet, Alison
ΤN
PA
     Amersham Biosciences UK Limited, UK
S0
     PCT Int. Appl., 53 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN. CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                              APPLICATION NO.
                                                                      DATE
PΤ
     WO 2004106923
                           A1
                                 20041209
                                              WO 2003-GB2323
                                                                      20030528
         W:
             AE, AG, AL,
                         AM, AT, AU, AZ,
                                           BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU,
                         CZ, DE, DK, DM,
                                           DZ,
                                               EC,
                                                   EE, ES,
                                                            FΙ,
                                                               GB, GD, GE, GH,
                                           JP,
             GM, HR, HU,
                          ID, IL,
                                  IN.
                                      IS,
                                               KE,
                                                   KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU,
                                  MD,
                                      MG,
                                                   MW, MX, MZ, NI, NO, NZ,
                         LV, MA,
                                           MK,
                                               MN,
                                                                            OM,
                                  SC,
             PH, PL, PT,
                         RO,
                             RU,
                                      SD,
                                           SE,
                                               SG,
                                                   SK,
                                                       SL,
                                                           TJ, TM,
                                                                    TN, TR,
                                                                            TT,
                                  VC,
                              UZ,
             TZ, UA, UG,
                          US,
                                      VN,
                                           YU,
                                               ZA,
                                                   ZM.
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     CA 2525685
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     AU 2003234038
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     CN 1839316
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                           Α
     JP 2006526137
                                 20061116
                                              JP 2005-500161
                                                                      20030528
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                                              US 2006-557521
     US 20070161116
                                 20070712
                           Α1
                                                                      20060911
                                 20030528
PRAI WO 2003-GB2323
     MARPAT 142:34835
0S
AB
     Disclosed are matched fluorescent reagents and a method for reproducibly
     labeling membrane components, such as those expressed on the cell surface,
     and subsequent differential anal. of the labeled components to detect
     differences between cell types and states. Furthermore, the present
     method utilizes an internal standard in order to match protein patterns across
     gels thereby avoiding gel-to-gel variation. The method according to the
     invention is particularly useful, for example, for detecting low abundance
     membrane proteins, for detecting changes in receptors expressed in the
     cell membrane, for example on ligand binding, or in response to stimuli.
IT
     644978-91-6 644978-92-7
     RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
        (differential anal. of cell surface proteins on closed membrane
        structures by labeling with dyes in presence of an internal standard)
RN
     644978-91-6 CAPLUS
     3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-
CN
```

yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RN

 $\begin{array}{lll} 644978-92-7 & \text{CAPLUS} \\ 3\text{H-Indolium,} & 2-\left[(1\text{E,3E,5E})-5-\left[1-\left[6-\left[\left[2-\left(2,5-\text{dihydro-2,5-dioxo-1H-pyrrol-1-y1}\right)\text{ethyl}\right]\text{amino}\right]-6-\text{oxohexyl}\right]-1, \\ 3-\text{dihydro-3,3-dimethyl-2H-indol-2-ylidene}]-1, \\ 3-\text{pentadien-1-yl}]-1, \\ 3, \\ 3-\text{trimethyl-5-sulfo-, inner salt} & \text{(CA INDEX NAME)} \end{array}$ CN

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD RE. CNT 5 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
     ANSWER 19 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
AN
     2004:1037349 CAPLUS
DN
     142:19000
ΤI
     Labeling of fusion proteins by enzymic incorporation of a coenzyme A
     derivative into an acyl carrier protein moiety
     Johnsson, Kai; George, Nathalie
ΤN
PA
     EPFL-Ecole Polytechnique Federale de Lausanne, Switz.
S0
     PCT Int. Appl., 46 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN. CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                              APPLICATION NO.
                                                                      DATE
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     WO 2004104588
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                                 20070530
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     ZA 2005009454
                           Α
                                                                      20051122
PRAI EP 2003-405364
                                 20030523
                           Α
     WO 2004-IB1733
                                 20040519
     CASREACT 142:19000; MARPAT 142:19000
0S
     A method for labeling acyl carrier protein (ACP) fusion proteins using
AB
     derivs. of CoA is described. The method relies on the transfer of a label
     from a CoA type substrate to an ACP fusion protein using a holo-acyl
     carrier protein synthase (ACPS) or a homolog thereof. The method allows
     detecting and manipulating the fusion protein, both in vitro and in vivo,
     by attaching mols, to the fusion proteins that introduce a new phys. or
     chemical property to the fusion protein. Examples of such labels are, among
     others, spectroscopic probes or reporter mols., affinity tags, mols.
     generating reactive radicals, cross-linkers, ligands mediating
     protein-protein interactions or mols. suitable for the immobilization of
     the fusion protein. Synthesis of a series of reporter mol. conjugates,
     including digoxigenin, Cy3 and Cy5, with CoA is reported.
     756898-09-6P 756898-10-9P
IT
     RL: ARU (Analytical role, unclassified); BUU (Biological use,
     unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL
     (Biological study); PREP (Preparation); USES (Uses)
         (preparation and labeling use of; labeling of fusion proteins by enzymic
        incorporation of coenzyme derivative into acyl carrier protein moiety)
RN
     756898-09-6 CAPLUS
     Coenzyme A, S-[1-[2-[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-
CN
     indol-2-ylidene)-1-propenyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-
     oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI)
     INDEX NAME)
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Absolute stereochemistry. Double bond geometry unknown.

PAGE 1-A

PAGE 1-B

RN

 $756898-10-9 \quad CAPLUS \\ Coenzyme A, \quad S-[1-[2-[[6-[2-[5-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1,3-pentadienyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl] amino] ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CARREY NAME)$ CNINDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

PAGE 1-A

IT 416853-49-1 616207-80-8

RL: RCT (Reactant); RACT (Reactant or reagent) (reactions of; labeling of fusion proteins by enzymic incorporation of coenzyme derivative into acyl carrier protein moiety)

RN 416853-49-1 CAPLUS

CN 3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

$$R - (CH_2)_5 - C - NH - CH_2 - CH_2 - N$$

RN 616207-80-8 CAPLUS

CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2004:775925 CAPLUS
- DN 141:421859
- TI Developing a peptide-based near-infrared molecular probe for protease sensing
- AU Pham, Wellington; Choi, Yongdoo; Weissleder, Ralph; Tung, Ching-Hsuan
- CS Center for Molecular Imaging Research, Massachusetts General Hospital, Harvard Medical School, Charlestown, MA, 02129, USA
- S0 Bioconjugate Chemistry (2004), 15(6), 1403-1407
- CODEN: BCCHES; ISSN: 1043-1802 PB American Chemical Society
- DT Journal
- LA English
- AB Recently near-IR (NIR) mol. probes have become important reporter mols. for a number of types of in vivo biomedical imaging. A peptide-based NIR fluorescence probe consisting of a NIR fluorescence emitter (Cy5.5), a NIR fluorescence absorber (NIRQ820), and a protease selective peptide sequence was designed to sense protease activity. Using a MMP-7 model, we showed that NIRQ820 efficiently absorbs the emission energy of Cy5.5 resulting in a low initial signal. Upon reacting with its target, MMP-7, the fluorescence signal of the designed probe was increased by 7-fold with a Kcat/Km of 100 000 M-1 s-1. The described synthetic strategy should have wide application for other NIR probe prepns.
- IT 795315-58-1P 795315-59-2P
 - RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
 - (peptide-based near-IR mol. probe for protease sensing)
- RN 795315-58-1 CAPLUS
- CN L-Cysteinamide, N-[[2-[3-[[5-carboxy-1, 3-dihydro-3, 3-dimethyl-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-chloro-1-cyclohexen-1-yl]ethenyl]-3, 3-dimethyl-1-(4-sulfobutyl)-3H-indolium-5-yl]carbonyl]glycyl-L-valyl-L-prolyl-L-leucyl-L-seryl-L-leucyl-L-threonyl-L-methionylglycyl-S-[1-[2-[[6-[2-[5-(3-ethyl-1, 3-dihydro-1, 1-dimethyl-6, 8-disulfo-2H-benz[e]indol-2-ylidene)-1, 3-pentadienyl]-1, 1-dimethyl-6, 8-disulfo-1H-benz[e]indolio]-1-oxohexyl]amino]ethyl]-2, 5-dioxo-3-pyrrolidinyl]-, bis(inner salt) (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

PAGE 1-C

RN 795315-59-2 CAPLUS

CN L-Cysteinamide, glycyl-L-seryl-L-methionyl-L-leucyl-L-prolyl-L-valyl-L-threonyl-L-leucylglycyl-S-[1-[2-[[6-[2-[5-(3-ethyl-1, 3-dihydro-1, 1-dimethyl-6, 8-disulfo-2H-benz[e]indol-2-ylidene)-1, 3-pentadienyl]-1, 1-dimethyl-6, 8-disulfo-1H-benz[e]indolio]-1-oxohexyl]amino]ethyl]-2, 5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 2-A

H2N

PAGE 2-B

RE. CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 21 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2004:714940 CAPLUS
- DN 141:391304
- TI General Strategy for Biosensor Design and Construction Employing Multifunctional Surface-Tethered Components
- AU Medintz, Igor L.; Anderson, George P.; Lassman, Michael E.; Goldman, Ellen R.; Bettencourt, Laura A.; Mauro, J. Matthew
- CS Center for Bio/Molecular Science and Engineering, U.S. Naval Research Laboratory, Washington, DC, 20375, USA
- SO Analytical Chemistry (2004), 76(19), 5620-5629 CODEN: ANCHAM; ISSN: 0003-2700
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 141:391304
- AB Biosensors function by reversibly linking bioreceptor-target analyte binding with closely integrated signal generation and can either continuously monitor analyte concns. or be returned to baseline readout values by removal of analyte. We present an approach for producing fully reversible, reagentless, self-assembling biosensors on surfaces. In the prototype biosensor, quencher-dye-labeled biotin-linked E. coli maltose binding protein (MBP) bound in a specific orientation to a NeutrAvidin-coated surface is employed as a bioreceptor. sensor formation, a modular tether arm consisting of a flexible biotinylated DNA oligonucleotide, a fluorescence resonance energy-transfer (FRET) donor dye, and a distal β -cyclodextrin (β -CD) analyte analog is bound in an equimolar amount to the same surface by means of DNA-directed immobilization. After self-assembly, a baseline level of FRET quenching is observed due to specific interaction between the β -CD of the flexible tether arm and the sugar binding site of MBP, which brings the two dyes into proximity. Addition of the target analyte, the nutrient maltose, displaces the linked $\beta\text{-CD-dye}$ of the DNA-based tether arm, and a concentration-dependent change in FRET results. Biosensor sensitivity and dynamic range can be controlled by either using MBP variants having different binding consts. or by binding of modulator DNA oligonucleotides that are complementary to the flexible DNA tether. The sensor can be regenerated and returned to baseline quenching levels by washing away analyte. A complex set of interactions apparently exists on the sensing surface that may contribute to sensor behavior and range. This approach may represent a general way to assemble a wide range of useful biosensors. 616207-80-8

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(general strategy for biosensor design and construction employing multifunctional surface-tethered components for maltose anal.)

- RN 616207-80-8 CAPLUS
- CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 22 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2004:534613 CAPLUS
- DN 141:256678
- TI Specific Labeling of Cell Surface Proteins with Chemically Diverse Compounds
- AU George, Nathalie; Pick, Horst; Vogel, Horst; Johnsson, Nils; Johnsson, Kai
- CS Institute of Chemical Sciences and Engineering, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, CH-1015, Switz.
- SO Journal of the American Chemical Society (2004), 126(29), 8896-8897 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- AB The specific and covalent labeling of fusion proteins with synthetic mols. opens up new ways to study protein function in the living cell. Here the authors present a novel method that allows for the specific and exclusive extracellular labeling of proteins on the surfaces of live cells with a large variety of synthetic mols. including fluorophores, protein ligands, or quantum dots. The approach is based on the specific labeling of fusion proteins of acyl carrier protein with synthetic mols. through post-translational modification catalyzed by phosphopantetheinetransferase. The specificity and versatility of the labeling should allow it to become an important tool for studying and manipulating cell surface proteins and for complementing existing approaches in cell surface engineering.
- IT 756898-09-6P 756898-10-9P
 - RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 - (diverse ligand preparation and use in
 - phosphopantetheinyltransferase-catalyzed labeling of cell surface proteins with acyl carrier protein fusion product derivs.)
- RN 756898-09-6 CAPLUS
- CN Coenzyme A, S-[1-[2-[[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1-propenyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

PAGE 1-A

RN

756898-10-9 CAPLUS Coenzyme A, S-[1-[2-[[6-[2-[5-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1,3-pentadienyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CA TYPEY NAME) CNINDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

416853-49-1 616207-80-8 IT

RL: RCT (Reactant); RACT (Reactant or reagent) (diverse ligand preparation and use in phosphopantetheinyltransferase-catalyzed labeling of cell surface proteins with acyl carrier protein fusion product derivs.)

RN

416853-49-1 CAPLUS
3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-yliden-1,3-pentadien-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt CN (CA INDEX NAME)

H03S Me Me CH-CH=CH-CH=CH
$$^{\rm N+}$$
 Me Me S03

RN 616207-80-8 CAPLUS

yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
    ANSWER 23 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
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2004:41759 CAPLUS AN

DN 140:90327

ΤI Cysteine-binding fluorescent cyanine dyes for saturation labelling of proteins and application in 2D-gel electrophoresis

Williams, Karen; Stone, Timothy; Simmonds, Adrian Christopher; Sweet, Alison Claire; Fowler, Susan Janet IN

PA Amersham Biosciences UK Limited, UK

S0 PCT Int. Appl., 58 pp. CODEN: PIXXD2

Patent DT

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1 7111.	FAN. CNT 1 PATENT NO.				KIND DATI		DATE		APPLICATION N			NO.		DATE				
PΙ	WO 2004005933			A1 20040115		WO 2002-GB3142						20020708						
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PRAI		2002						2002	0708									
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GI																		

AB A matched set of fluorescent dyes is provided, wherein each dye of the set is capable of covalent attachment to a protein and wherein each of the dyes has a mol. structure and a charge that is matched one with the other, such that relative electrophoretic mobility of a protein labeled with one dye of the set is the same as the electrophoretic mobility of the protein labeled with a different dye of the set. The matched set comprises at least two different fluorescent dyes of formula (I): wherein n is 1, 2, or 3; Z1 and Z2 independently represent the carbon atoms necessary to complete a Ph or naphthyl ring system; one of groups R1 and R2 is a target bonding group; remaining group R1 or R2 is selected from -(CH2)4-W or -(CH2)r-H; group R3 is hydrogen, except when either R1 or R2 is -(CH2)r-H, in which case R3 is W; and W is selected from sulfonic acid and sulfonate. The invention also provides a method for saturation labeling of a protein with a fluorescent dye so as to label all available target amino acid, suitably

Ι

cysteine, residues in the protein, thereby giving a single population of labeled protein mols.

IT 644978-91-6P 644978-92-7P 644978-93-8P 644978-94-9P 644978-95-0P 644978-96-1P 644978-97-2P 644978-98-3P 644978-99-4P 644979-00-0P 644979-01-1P

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (cysteine-binding fluorescent cyanine dyes for saturation labeling of proteins and application in 2D-gel electrophoresis)

RN 644978-91-6 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3, 3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 644978-92-7 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-1,3,3-trimethyl-5-sulfo-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 644978-93-8 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1-propen-1-yl]-3, 3-dimethyl-1-propyl-5-sulfo-, inner salt (CA INDEX NAME)

RN 644978-94-9 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1, 3-pentadien-1-yl]-1-ethyl-3, 3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 644978-95-0 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[5-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-5-oxopentyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RN 644978-96-1 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1-propen-1-yl]-3, 3-dimethyl-1-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 644978-97-2 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[5-[[2-(2, 5-dihydro-2, 5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-5-oxopentyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1, 3-pentadien-1-yl]-3, 3-dimethyl-1-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 644978-98-3 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[3-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)propyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 644978-99-4 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E)-3-[1-[6-[[3-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)propyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1-propen-1-yl]-3,3-dimethyl-1-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 644979-00-0 CAPLUS

CN 3H-Indolium, 2-[(1E, 3E, 5E)-5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3,3-dimethyl-1-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN

 $\begin{array}{lll} 644979-01-1 & CAPLUS\\ 3H-Indolium, & 2-[(1E,3E)-3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1, 3-dihydro-3, 3-dimethyl-2H-indol-2-ylidene]-1-propen-1-yl]-1, 3, 3-trimethyl-5-sulfo-, inner salt (CA INDEX NAME) \end{array}$ CN

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD RE. CNT 4 ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 24 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2003:679367 CAPLUS
- DN 139:334980
- TI A fluorescence resonance energy transfer sensor based on maltose binding protein
- AU Medintz, Igor L.; Goldman, Ellen R.; Lassman, Michael E.; Mauro, J. Matthew
- CS Center for Bio/Molecular Science and Engineering, U.S. Naval Research Laboratory, Washington, DC, 20375, USA
- SO Bioconjugate Chemistry (2003), 14(5), 909-918 CODEN: BCCHES; ISSN: 1043-1802
- PB American Chemical Society
- DT Journal
- LA English
- AB A fluorescence resonance energy-transfer (FRET) sensing system for maltose based on E. coli maltose binding protein (MBP) is demonstrated. The FRET donor portion of the sensing system consists of MBP modified with long wavelength-excitable cyanine dyes (Cy3 or Cy3.5). The novel acceptor portion of the sensor consists of β -cyclodextrin (β -CD) modified with either the cyanine dye Cy5 or the dark quencher QSY9. Binding of the modified β -CD to dye-conjugated MBP results in assembly of the FRET complex. Added maltose displaces the β -CD-dye adduct and disrupts the FRET complex, resulting in a direct change in fluorescence of the donor moiety. In the use of these FRET pairs, MBP dissociation values for maltose were estimated (0.14-2.90 μ M). Maltose limits of detection were in the 50-100 nm range.
- IT 616207-80-8
 - RL: ARU (Analytical role, unclassified); ANST (Analytical study) (electron acceptor; fluorescence resonance energy transfer sensor based on maltose binding protein)
- RN 616207-80-8 CAPLUS
- CN 3H-Indolium, 2-[3-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propen-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2002:135291 CAPLUS
- DN 136:337160
- TI Imaging of the fluorescence spectrum of a single fluorescent molecule by prism-based spectroscopy
- AU Suzuki, Yoshikazu; Tani, Tomomi; Sutoh, Kazuo; Kamimura, Shinji
- CS Department of Life Sciences, University of Tokyo, Graduate School of Arts and Sciences, Tokyo, Meguro, 153-8902, Japan
- SO FEBS Letters (2002), 512(1-3), 235-239 CODEN: FEBLAL; ISSN: 0014-5793
- PB Elsevier Science B.V.
- DT Journal
- LA English
- AB We have devised a novel method to visualize the fluorescence spectrum of a single fluorescent mol. using prism-based spectroscopy. Equiping a total internal reflection microscope with a newly designed wedge prism, we obtained a spectral image of a single rhodamine red mol. attached to an essential light chain of myosin. We also obtained a spectral image of single-pair fluorescence resonance energy transfer between rhodamine red and Cy5 in a double-labeled myosin motor domain. This method could become a useful tool to investigate the dynamic processes of biomols. at the single-mol. level.
- IT 416853-49-1
 - RL: ARU (Analytical role, unclassified); PRP (Properties); ANST (Analytical study)
 - (imaging of fluorescence spectrum of single fluorescent mol. by prism-based spectroscopy)
- RN 416853-49-1 CAPLUS
- CN 3H-Indolium, 2-[5-[1-[6-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (CA INDEX NAME)

RE. CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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